

Fractional Inversion in Krylov Space

B. Bunk ^a *

^aInstitut für Physik, Humboldt–Universität zu Berlin, Invalidenstr.110, D–10115 Berlin, Germany

The fractional inverse $M^{-\gamma}$ (real $\gamma > 0$) of a matrix M is expanded in a series of Gegenbauer polynomials. If the spectrum of M is confined to an ellipse not including the origin, convergence is exponential, with the same rate as for Chebyshev inversion. The approximants can be improved recursively and lead to an iterative solver for $M^\gamma x = b$ in Krylov space. In case of $\gamma = 1/2$, the expansion is in terms of Legendre polynomials, and rigorous bounds for the truncation error are derived.

1. Gegenbauer Polynomials

The key relation is the generating function

$$(1 + t^2 - 2tz)^{-\gamma} = \sum_{n=0}^{\infty} t^n C_n^\gamma(z) \quad (1)$$

with a real parameter $\gamma > 0$. It defines the Gegenbauer polynomials $C_n^\gamma(z)$, see [1], part 10.9. They obey the recursion relation

$$(n+1)C_{n+1}^\gamma(z) + (n+2\gamma-1)C_{n-1}^\gamma(z) = 2(n+\gamma)zC_n^\gamma(z) \quad (2)$$

($n \geq 0$, $C_{-1}^\gamma = 0$) and are normalised such that

$$C_n^\gamma(1) = \frac{\Gamma(2\gamma+n)}{n!\Gamma(2\gamma)}. \quad (3)$$

Special cases are the Legendre polynomials

$$C_n^{1/2}(z) = P_n(z) \quad (4)$$

and the Chebyshev polynomials of the second kind

$$C_n^1(z) = U_n(z). \quad (5)$$

Estimates of C_n^γ are obtained with the aid of the integral representation

$$C_n^\gamma(z) = \frac{2^{1-2\gamma}\Gamma(2\gamma+n)}{n!\Gamma(\gamma)^2} \int_0^\pi d\varphi (\sin \varphi)^{2\gamma-1} (z + \sqrt{z^2-1} \cos \varphi)^n. \quad (6)$$

2. Convergence of Gegenbauer expansions

The relation (1) was introduced to define the Gegenbauer polynomials, but it also serves as an efficient expansion of $(1 + t^2 - 2tz)^{-\gamma}$ in polynomials of z . In this context, the relative error of the truncated series is of particular importance:

$$R_n(z) = 1 - (1 + t^2 - 2tz)^\gamma \sum_{k=0}^n t^k C_k^\gamma(z) \quad (7)$$

$$= (1 + t^2 - 2tz)^\gamma \sum_{k=n+1}^{\infty} t^k C_k^\gamma(z) \quad (8)$$

On the line segment $z \in [-1, 1]$, the Gegenbauer polynomials are uniformly bounded by

$$\begin{aligned} |C_n^\gamma(z)| &\leq C_n^\gamma(1) \quad \text{for } z \in [-1, 1] \\ &\simeq \frac{n^{2\gamma-1}}{\Gamma(2\gamma)} \quad \text{as } n \rightarrow \infty \end{aligned} \quad (9)$$

Therefore the expansion (1) converges uniformly in z , provided that $|t| < 1$. The relative error (8) decreases like

$$|R_n(z)| = \mathcal{O}(|t|^{n+1}), \quad (10)$$

possibly up to powers of n . For the Legendre case ($\gamma = 1/2$), the following rigorous estimate is proven in [2]:

$$|R_n(z)| \leq |t|^{n+1} \quad \text{for } z \in [-1, 1]. \quad (11)$$

To extend these considerations to $z \notin [-1, 1]$, it is convenient to parametrise the complex plane in terms of confocal ellipses (as in the case of Chebyshev polynomials, see [3,4]). Inside the ellipse

$$z = \cosh(\theta + i\phi), \quad \theta \geq 0, \quad \phi \in [0, 2\pi] \quad (12)$$

*email: bunk@physik.hu-berlin.de

C_n^γ is bounded by

$$\begin{aligned} |C_n^\gamma(z)| &\leq C_n^\gamma(\cosh \theta) \\ &\leq C_n^\gamma(1) \cosh n\theta \end{aligned} \quad (13)$$

and convergence of the expansion (1) is uniform in z if $|t|e^\theta < 1$. We also have

$$|R_n(z)| = \mathcal{O}(|t|e^\theta)^{n+1} \quad (14)$$

and for $\gamma = 1/2$ the general bound[2]

$$|R_n(z)| \leq (|t|e^\theta)^{n+1}. \quad (15)$$

3. Iterative solver

The aim is to solve

$$M^\gamma x = b \quad (16)$$

approximately in Krylov space, i.e. in terms of polynomials of M acting on b . To this end, parametrise M as

$$M = c(1 + t^2 - 2tA) \quad (17)$$

with $c, t \in \mathbb{C}$. If M has a spectrum on a line away from the origin, we can find a transformation with $|t| < 1$ such that $\text{spec} A \subset [-1, 1]$. More generally, if the spectrum of M is bounded by an ellipse which does not include the origin, it can be mapped into an ellipse (12) with $|t|e^\theta < 1$. In any case, $|t|$ resp. $|t|e^\theta$ should be as small as possible for optimal convergence.

The formal solution

$$x = c^{-\gamma}(1 + t^2 - 2tA)^{-\gamma} b \quad (18)$$

suggests to insert the Gegenbauer expansion (1) and to form the approximants

$$x_n = c^{-\gamma} \sum_{k=0}^n t^k C_k^\gamma(A) b = \sum_{k=0}^n t^k s_k. \quad (19)$$

The shifts

$$s_n \equiv c^{-\gamma} C_n^\gamma(A) b \quad (20)$$

inherit the recursion relation (2):

$$\begin{aligned} (n+1)s_{n+1} + (n+2\gamma-1)s_{n-1} \\ = 2(n+\gamma)As_n \end{aligned} \quad (21)$$

($n \geq 0$) to be started from

$$\begin{aligned} s_{-1} &= 0 \\ s_0 &= c^{-\gamma} b. \end{aligned}$$

As to the stability of the recursion, the error δs_n evolves for large n according to the approximate relation

$$\delta s_{n+1} + \delta s_{n-1} = 2A \delta s_n.$$

Consider an eigenvalue λ of A and express it as $\lambda = \cosh(\vartheta + i\varphi)$ with $0 \leq \vartheta \leq \theta$. Then the error of the corresponding mode of s_n behaves like

$$\delta s_n \propto e^{\pm(\vartheta+i\varphi)n}.$$

Note that the shifts s_n are to be multiplied by t^n when accumulated for the solution (19). Therefore, the modes of iterated errors in $t^n \delta s_n$ contribute $\sim (|t|e^{\pm\vartheta})^n \leq (|t|e^\theta)^n$, i.e. error propagation is damped due to $|t|e^\theta < 1$.

In conclusion, the recursion (21) provides a stable solver (19) for the linear problem (16). This was confirmed in a first application[5] within the boson algorithm for dynamical fermions.

A peculiar feature of this solver is that it cannot be started from an arbitrary vector x , but only from $x_{-1} = 0$ or $x_0 = s_0$ as stated above. This is due to the fact that $M^\gamma x_{-1}$ cannot be evaluated for arbitrary x_{-1} (which is needed to bring the start vector to the r.h.s. of the equation). If an approximant x_n is to be improved in further iterations, the last shifts s_{n-1}, s_n have to be saved as well.

4. Error estimates

The rest vector and the relative error of x_n are both controlled by R_n eq.(8):

$$r_n = b - M^\gamma x_n = R_n(A) b \quad (22)$$

$$x - x_n = M^{-\gamma} r_n = R_n(A) x \quad (23)$$

Note that, in contrast to the case of plain inversion ($\gamma = 1$), r_n is not available during the iterative process, because M^γ is not computable for fractional γ . Therefore mathematical bounds for $\|R_n(A)\|$ are important to estimate the quality of the approximation. (Throughout this paper, $\|\cdot\|$

designates the Euclidean norm for vectors and the induced matrix norm.)

If M is normal, i.e. $[M, M^\dagger] = 0$, the same is true for A , and $\|R_n(A)\|$ is determined by the spectrum of A . This results in an estimate for the relative error

$$\begin{aligned} \|x - x_n\|/\|x\| &\leq \|R_{n+1}(A)\| \\ &= \max_i |R_n(\lambda_i(A))|. \end{aligned} \quad (24)$$

At this point, uniform bounds like (11) or (15) over the spectrum of A are useful. So far, they are available for $\gamma = 1/2$ only.

As an example, let $M = M^\dagger$ be positive definite with $\text{spec}M \subset [\lambda_{\min}, \lambda_{\max}]$. c and t are chosen such that eq.(17) maps $M = \lambda_{\max} \rightarrow A = -1$ and $M = \lambda_{\min} \rightarrow A = 1$. This implies

$$\begin{aligned} \kappa &\equiv \frac{\lambda_{\max}}{\lambda_{\min}} = \left(\frac{1+t}{1-t} \right)^2 \\ \Rightarrow t &= \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \end{aligned}$$

Eq.(10) shows that t is the convergence factor, and it agrees with the one for optimal Chebyshev inversion and the bound for the Conjugate Gradient solver.

If $\text{spec}M$ is not known, one may proceed as follows: define A , based on a guess about the spectrum, and monitor the norm of the shifts $\|s_n\|$. The estimate

$$\begin{aligned} \|s_n\|/\|s_0\| &= \|C_n^\gamma(A)b\|/\|b\| \\ &\leq \|C_n^\gamma(A)\| \\ &\leq C_n^\gamma(\cosh \theta) \end{aligned} \quad (25)$$

is assumed to be saturated for large n , and this allows for a (pragmatic) determination of θ . If $|t|e^\theta \geq 1$, there will be no convergence and one has to stop and try again. Otherwise, θ is employed in the error estimate. It may also help to refine the parametrisation of M (choice of c and t) for later use.

5. Conclusions

- The Gegenbauer expansion allows to construct iterative solvers for $M^\gamma x = b$ with the same rate of convergence as (optimal) Chebyshev methods for $\gamma = 1$.

- If the spectrum of M is known, the relative error of the approximation can be estimated. Tight bounds are known for $\gamma = 1/2$.
- If the spectrum is uncertain, the growth of the shift vectors can be used for a rough estimate.
- Polynomial approximations $\mathbf{P}_n(M) \approx M^{-\gamma}$ are obtained along the same lines.
- The polynomials generated by the Gegenbauer expansion are not optimal in any sense, but the method is distinguished by its conceptual and computational simplicity.

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